Determination of Complex Surface Reconstructions: Geometric Structure of Strained Ag Films on Ru(0001)

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We present an x-ray scattering study of the interfacial structure of thin strained Ag films on Ru(0001) surfaces at 690 K. Our results give new insight into the structural details and the mechanisms of strain accommodation at this bimetallic interface. The origin of the strain arises from a lattice mismatch accompanying epitaxy with a 6.3% compressive strain for Ag on Ru.

The analysis of 317 independent in- and out-of-plane reflections reveals a (20x20) reconstruction of the Ag layer. The motive of the superstructure is dominated by an extended two-dimensional dislocation pattern, which separates smaller regions of fcc and hcp stacking with the Ru substrate (Figure 1(a)). The details of this complex reconstruction are described by a set of two-dimensional modulation functions that can be used to calculate the strain distribution on an atomic level. Through the reconstruction, the theoretical lattice misfit of -6.3% is reduced to an average value of -3%. The calculated strain distribution is highly inhomogeneous and peaks in an orthogonal network of ridges of strain with unit cell dimensions (Figure 1(b)). The analysis of our out-of-plane data suggests that the corrugation of the Ag layer follows a hard-ball model indicating a weak ad-layer substrate interaction. Its distance to the underlying Ru substrate is homogeneously compressed by 1.8% with respect to the Ru ***c*** lattice constant. We find no indication that the Ru layers reconstruct laterally. However, the first two Ru layer distances are slightly compressed.

The analysis of this reconstruction was accomplished by the application of very fast simulated re-annealing algorithms.

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References: [1] H. Zajonz et al., *Phys. Rev. B* **62** (15) *10436*, 2000